Chocolates classification according to their volatile compounds fingerprints measured by PTR-ToF-MS

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Dark chocolates develop several organoleptic characteristics depending on cocoa origin, cocoa variety and fabrication process. These parameters influence the chemical composition of the chocolates, and among other components volatile organic compounds (VOCs) responsible for aroma mainly determine their sensory perception. Sensory evaluation is able to discriminate chocolates with various organoleptic properties. Proton Transfer Reaction Mass Spectrometry (PTR-MS) is capable of monitoring VOCs released in foodstuffs headspace at ppb level in real time. But is PTR-MS able to discriminate chocolates as sensory analysis does?

To answer this question, 192 dark chocolates produced from cocoa beans of different variety and origin but with the same fabrication process were investigated. A preliminary sensory analysis performed on this set of chocolates classified them into four sensory poles. VOCs emitted from the 192 samples were analyzed by dynamic headspace coupled to a PTR-Time of Flight (ToF)-MS instrument. The headspace analyses of 1g of chocolate mixed under stirring with 1mL of artificial saliva contained in 20mL vials equilibrated at 36.2°C for 2 hours were performed in triplicate. The average areas under the curves obtained for the 2mn release of each of the significant 314 ions present in the mass spectra were used to perform unsupervised (Principal Component Analysis PCA) and supervised (Partial Least-Square Discriminant Analysis PLS-DA) multivariate data analyses to explore and represent samples and variables.

Results showed that among the 314 ions studied, all present in the 192 samples, 46 were not discriminant. Ion intensities were higher in sensory poles 1 and 2. The produced "chemical maps" showed that the headspace analyses of the chocolates allowed discrimination between the four sensory poles. Finally, by comparing the chemical fingerprints to the sensory ones, it appeared that sensory classification of the 192 chocolates could be explained by the profiles of flavour compounds released by the matrix.